

# HW6 Bio3D

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## Input

The function inputs structures of same or different proteins under different biological states of drug bound or not. In detail the inputs examines selected protein chain and atom types to analyze.

## Purpose

The function performed with the process of extracting the B-factors from multiple PDB structures and plotting them for direct comparison. As the B-factor reflect atomic mobility within the protein, examination of it can visualizes the structural flexibility differences in protein-drug interactions.

## Output

The output are B-factor vs resdue number plots where peaks/higher B-factors correlates to a higher degree of flexibility in a certain region. The multiple plots of kinase with drug or not and different kinase help us understand the impact to stabilitzation of the protein structure from the drug binding.

```
library(bio3d)

plot_bfactors <- function(pdb_ids, chain = "A", eley = "CA") {
  if (!is.character(pdb_ids)) stop("pdb_ids must be a character vector.")

  b_list <- list()

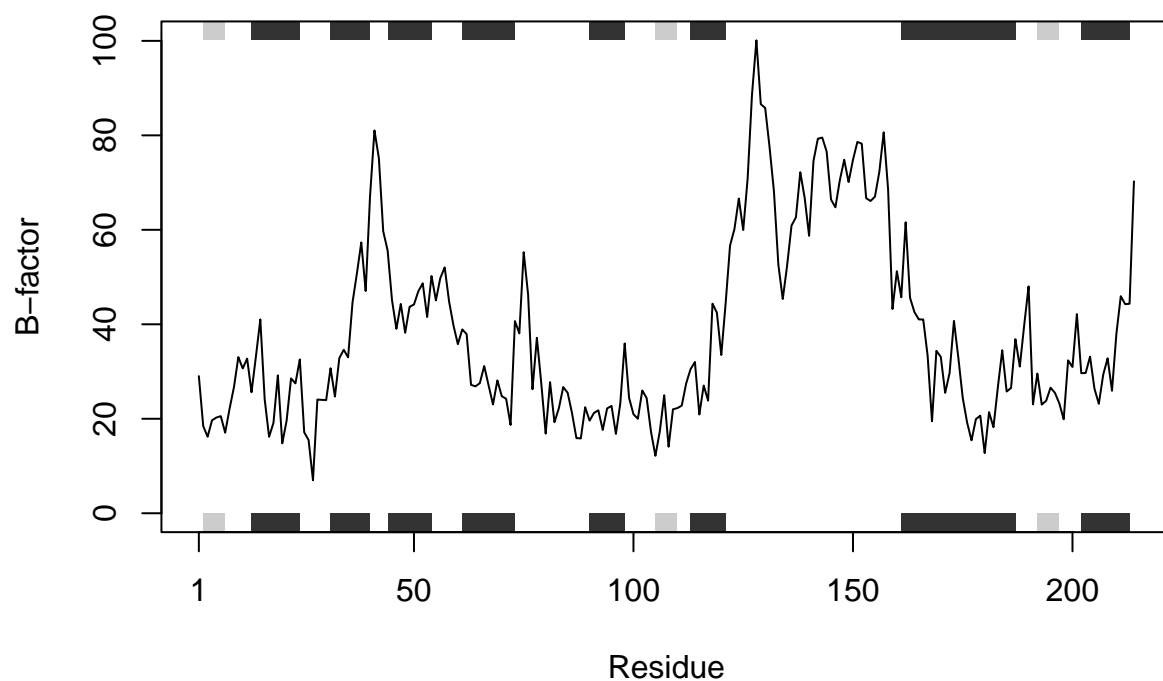
  for (id in pdb_ids) {
    pdb <- read.pdb(id)
    pdb_trim <- trim.pdb(pdb, chain = chain, eley = eley)
    b_vals <- pdb_trim$atom$b
    b_list[[id]] <- b_vals
    plotb3(b_vals,
           sse = pdb_trim,
           typ = "l",
           ylab = "B-factor",
           main = paste("B-factor profile:", id))
  }
  invisible(b_list)
}
```

Run the examples:

```
plot_bfactors(c("4AKE", "1AKE", "1E4Y"))
```

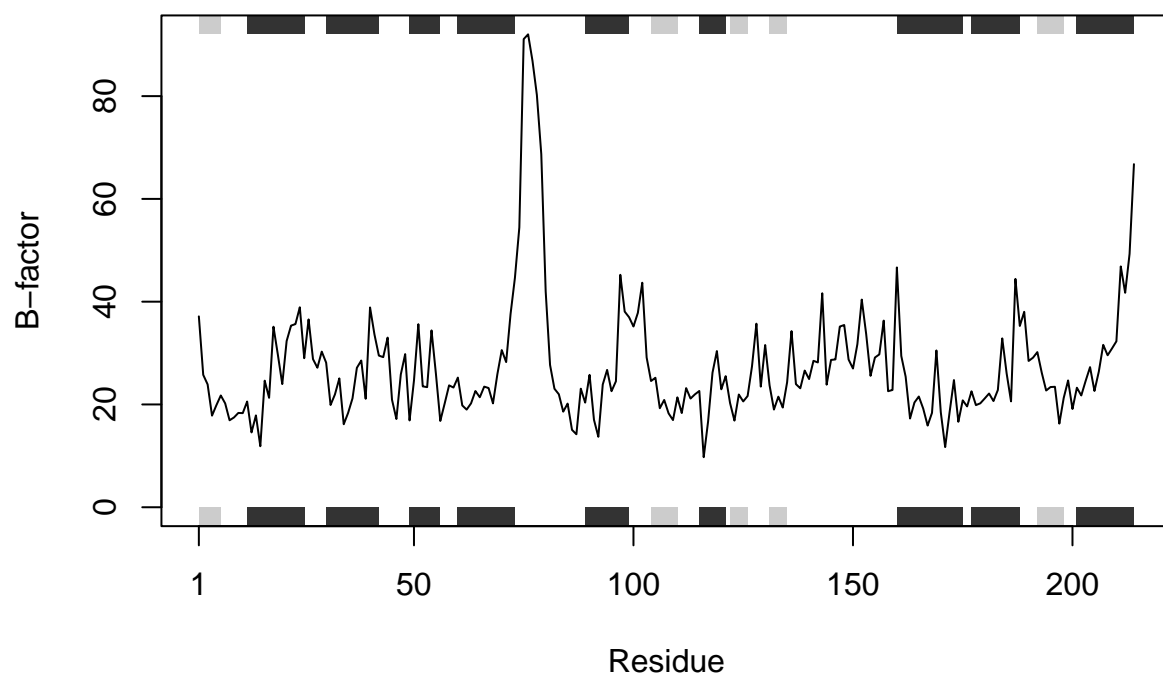
```
## Note: Accessing on-line PDB file
```

### B-factor profile: 4AKE



```
## Note: Accessing on-line PDB file
## PDB has ALT records, taking A only, rm.alt=TRUE
```

### B-factor profile: 1AKE



## Note: Accessing on-line PDB file

**B-factor profile: 1E4Y**

